Nicosulfuron 111991-09-4 | DTXSID6034764

Model	Performance
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Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 3.61

Global applicability domain: Outside

Local applicability domain index: 1.97e-01

Confidence level: 6.56e-01

Nearest Neighbors from the Training Set

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Malaoxon

Measured: 1.12 Predicted: 1.49

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Tris(2-hydroxyethyl) isocyanurate

Measured: 1.58 Predicted: 1.61

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N,N,N',N',N",N"-

Hexakis(methoxymethyl)-1,3,5-triazine-2,4,6-triamine

Measured: 3.47 Predicted: 4.50

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Tris(2-butoxyethyl) phosphate

Measured: 5.75 Predicted: 6.32

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Malathion
Measured: 33.1
Predicted: 21.9